A tractable Multi-Partitions Clustering

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Outline

Data

$\mathbf{x} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$ composed of n independent observations $\boldsymbol{x}_i = (x_{i1}, \ldots, x_{id})$ defined on $\mathbb{R}^d$.

Goal

Cluster the data in G clusters.

What variables use in clustering?

- Well-posed problem in the supervised classification setting with objective criteria: error rate, AUC, ...
- Ill-posed problem in clustering since the class variable is not known by advance. Thus, what are the most relevant variables with respect to this unknown variable?
- Pragmatic solution 1: Prior choice of the practitioner among available variables (according to some focus)
- Pragmatic solution 2: Posterior analysis of the correlation between the predicted cluster (based on all the variables) and each variable

The model based clustering solution

- Mixture models allow to perform clustering by modelling the distribution of the data as a mixture of G components each one corresponding to a cluster.
- Thus possibility to suppose that some variables do not depend (directly) on the cluster in the probabilistic model.

Some references

- Raftery & Dean (2006): some classifying, and some redundant variables. Redundant variables independent of the cluster given the classifying variables.
- Maugis & *al.* (2009): refinement of Raftery & Dean (2006) by specifying the role of each variable (classifying, redundant or independant).

Advantages of these approaches

- Improve the accuracy of the clustering by decreasing the variance of the estimators.
- Allow some specific interpretation of the classifying variables.

Limitations of these approaches

- Combinatorial problem to select the best model with these refined approaches
- Search too hard to perform when the number of variables is large

Solution: use simpler models for a better search (Marbac & Serdki 2016,2017)

- Assumption of conditional independence of the classifying variables given the cluster
- Non-classifying variables are independent
- Optimisation of the integrated classification likelihood (ICL)
- Better results than previous approaches on large number of variables with moderated sample size
- The independence assumption allows to easily consider the heterogeneous data setting

Several clustering variables

- The variables in the data can convey several clustering view points with respect to different groups of variables
- Allow to find some clustering which could be hidden by other variables

Some references

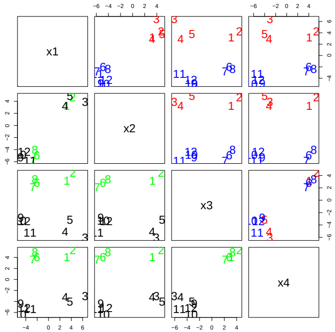
- Galimberti & *al.* (2007): First proposition of a multiple Gaussian mixture model
- Galimberti & *al.* (2017): Refinement of the previous model with ideas similar to to Raftery & Dean (2006) et Maugis & *al.* (2009)

Remarks

- Smart modelling of the role of each variable
- Search hard to perform when the number of variables is large
- Specific to the Gaussian setting

Illustration of a multiple partition

id	x_1	x_2	x_3	x_4	z_1	z_2
1	3.23	3.28	3.14	4.08	1	1
2	4.26	4.7	4.41	5.36	1	1
3	6.43	3.94	-6.09	-3.03	1	2
4	2.93	3.22	-5.05	-3.2	1	2
5	3.77	4.88	-3.21	-4	1	2
6	-2.03	-4.9	2.81	4	2	1
7	-2.78	-5.87	2.11	3.57	2	1
8	-2.38	-4.06	3.35	4.91	2	1
9	-4.88	-5.26	-2.86	-4.42	2	2
10	-5.01	-4.83	-3.3	-6.42	2	2
11	-3.25	-5.84	-5.23	-5.35	2	2
12	-4.28	-4.36	-3.38	-5.14	2	2



Main assumptions

- The variables can be decomposed in B independent blocks.
- The block b follows a mixture with G_b components (for $b = 1, \dots, B$), with the assumption of class conditional independence of the variables.

Notations

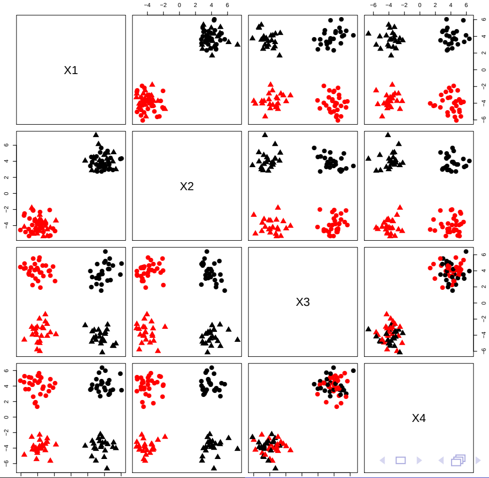
- $\boldsymbol{\omega} = (\omega_j; j = 1, \dots, d)$ the repartition of the variables in blocks; $\omega_j = b$ if variable j belongs to block b.
- $\boldsymbol{m} = (G_1, \dots, G_B, \boldsymbol{\omega})$ defines the model
- $\Omega_b = \{j : \omega_j = b\}$ the subset of variables belonging to block b
- $\boldsymbol{\theta} = (\boldsymbol{\pi}, \boldsymbol{\alpha})$ model parameters
- $p(.|\boldsymbol{\alpha}_{jg})$ the pdf of the distribution of parameters $\boldsymbol{\alpha}_{jg}$.

Probability distribution function of $\boldsymbol{x}_i$

$$p(\boldsymbol{x}_i|\boldsymbol{m},\boldsymbol{\theta}) = \prod_{b=1}^{B} p(\boldsymbol{x}_{i\{b\}}|\boldsymbol{m},\boldsymbol{\theta}) \text{ with } p(\boldsymbol{x}_{i\{b\}}|\boldsymbol{m},\boldsymbol{\theta}) = \sum_{g=1}^{G_b} \pi_{bg} \prod_{j\in\Omega_b} p(x_{ij}|\boldsymbol{\alpha}_{jg}),$$

Illustration :

- $n = 100$ from a MPM with $B = 2$ blocks of two variables.
- Variable 1 and 2 belong to block 1 and variables 3 and 4 in block 2
- Each block follows a bi-component Gaussian mixture (*i.e.*, $G_b = 2$) with equal proportions (*i.e.*, $\pi_{bg} = 1/2$) and $\mu_{j1} = 4$, $\mu_{j2} = -4$ and $\sigma_{jg} = 1$.



Remarks

- Different partitions explained by subsets of variables.
- Generalizes approaches used for variable selection in model-based clustering (if $B = 2$ and $G_1 = 1$ then variables belonging to block 1 are not relevant for the clustering, while variables belonging to block 2 are relevant)
- MGMM permits **variable selection** and **multiple partitions** explained by **subsets of variables** (variables classification).
- Sparse model: number of parameters $\nu_{\boldsymbol{m}} = \sum_{b=1}^{B}(G_b - 1) + G_b \sum_{j\in\Omega_b} \nu_j$
- Better model search expected than in the model of Galimberti & *al.* (2017)
- Natural extension to the heterogeneous data setting

Identifiability

Model identifiability is directly obtained from the identifiability of Gaussian mixture with local independence (Teicher, 1963, 1967).

Observed-data likelihood for sample x and model m

$$\ell(\boldsymbol{\theta}|\boldsymbol{m},\mathbf{x}) = \sum_{b=1}^{B}\sum_{i=1}^{n}\ln\left(\sum_{g=1}^{G_b}\pi_{bg}\prod_{j\in\Omega_b}p(x_{ij}|\boldsymbol{\alpha}_{jg})\right).$$

Latent partitions

- B independent mixtures
- $\mathbf{z} = (\boldsymbol{z}_{ib}; i=1,\dots,n; b=1,\dots,B)$ vectors of the component memberships
- $\boldsymbol{z}_{ib} = (z_{ib1},\dots,z_{ibG_b})$ where $z_{ibg}=1$ if observation i arose from component g for block b, and $z_{ibg}=0$ otherwise

Completed-data likelihood for sample x and model m

$$\ell(\boldsymbol{\theta}|\boldsymbol{m},\mathbf{x},\mathbf{z}) = \sum_{b=1}^{B}\ln p(\mathbf{z}_b|\boldsymbol{\pi}_b) + \sum_{j=1}^{d}\ln p(\mathbf{x}_j|\mathbf{z}_{\omega_j},\boldsymbol{\alpha}_j),$$

where $\ln p(\mathbf{z}_b|\boldsymbol{\pi}_b) = \sum_{i=1}^{n}\sum_{g=1}^{G_b} z_{ibg}\ln\pi_{bg}$ and
$\ln p(\mathbf{x}_j|\mathbf{z}_b,\boldsymbol{\alpha}_j) = \sum_{i=1}^{n}\sum_{g=1}^{G_b} z_{ibg}\ln p(x_{ij}|\boldsymbol{\alpha}_{jg})$.

EM algorithm

Starting from the initial value $\boldsymbol{\theta}^{[0]}$, iteration $[r]$ is composed of two steps:
E-step Computation of the fuzzy partitions $t_{ibg}^{[r]} := \mathbb{E}[Z_{ibg}|\boldsymbol{x}_{i\{b\}}, \boldsymbol{m}, \boldsymbol{\theta}^{[r-1]}]$, hence for $b = 1, \dots, B$, for $g = 1, \dots, G_b$, for $i = 1, \dots, n$

$$t_{ibg}^{[r]} = \frac{\pi_{bg}^{[r-1]} \prod_{j \in \Omega_b} p(x_{ij}|\boldsymbol{\alpha}_{jg}^{[r-1]})}{\sum_{k=1}^{G_b} \pi_{bk}^{[r-1]} \prod_{j \in \Omega_b} p(x_{ij}|\boldsymbol{\alpha}_{jg}^{[r-1]})},$$

M-step Maximization of the expected value of the complete-data log-likelihood over the parameters,

$$\pi_{bg}^{[r]} = \frac{n_{bg}^{[r]}}{n} \text{ and } \boldsymbol{\alpha}_{jg}^{[r]} = \arg\max_{\boldsymbol{\alpha}_{jg} \in \Theta_j} Q(\boldsymbol{\alpha}_{jg}|\mathbf{x}_j, \mathbf{t}_{\omega_j g}^{[r]}),$$

where $Q(\boldsymbol{\alpha}_{jg}|\mathbf{x}_j, \mathbf{t}_b) = \sum_{i=1}^{n} t_{ibg} \ln p(x_{ij}|\boldsymbol{\alpha}_{jg})$.

Remarks

- Independence between the B blocks of variables permits to maximize the observed-data log-likelihood on each block separately.
- Possible modification to perform the block estimation and the parameter inference simultaneously.
- In practice the number of blocks, the repartition of variables into blocks, and the number of classes per block are unknown.

Model collection $\mathcal{M}$

$$\mathcal{M} = \{\boldsymbol{m} : \omega_j \leq B_{\max} \text{ and } G_b \leq G_{\max}; j = 1, \dots, d; b = 1, \dots, B_{\max}\},$$

where $B_{\max}$ is the maximum number of blocks and $G_{\max}$ is the maximum number of components within block.

Model selection

Model selection often achieved by searching the model $\boldsymbol{m}^\star$ maximizing the BIC criterion which is defined by

$$\text{BIC}(\boldsymbol{m}) = \max_{\boldsymbol{\theta_m}} \ell_{pen}(\boldsymbol{\theta_m}|\boldsymbol{m}, \mathbf{x})$$

where

$$\ell_{pen}(\boldsymbol{\theta_m}|\boldsymbol{m}, \mathbf{x}) = \ell(\boldsymbol{\theta_m}|\boldsymbol{m}, \mathbf{x}) - \frac{\nu_{\boldsymbol{m}}}{2} \ln n.$$

Remark

$$(\boldsymbol{m}^\star, \hat{\boldsymbol{\theta}}_{\boldsymbol{m}^\star}) = \arg\max_{(\boldsymbol{m}, \boldsymbol{\theta_m})} \ell_{pen}(\boldsymbol{\theta_m}|\boldsymbol{m}, \mathbf{x})$$

Penalised completed likelihood

$$\ell_{pen}(\boldsymbol{\theta}_{\boldsymbol{m}}|\boldsymbol{m},\mathbf{x},\mathbf{z}) = \ell(\boldsymbol{\theta}_{\boldsymbol{m}}|\boldsymbol{m},\mathbf{x},\mathbf{z}) - \frac{\boldsymbol{\nu}_{\boldsymbol{m}}}{2}\log n$$
$$= \sum_{b=1}^{B} \ln p(\mathbf{z}_b|\boldsymbol{\pi}_b) - \frac{G_b - 1}{2}\ln n + \sum_{j=1}^{d} \ln p(\mathbf{x}_j|\mathbf{z}_{\omega_j},\boldsymbol{\alpha}_j) - \frac{\nu_j G_{\omega_j}}{2}\ln n,$$

Consequence

- For $\mathbf{z}_b$ fixed: possibility to re-affect each variable **individually** to the most accurate block.
- Thus computationnaly attractive

Combinatorial model selection through a modified the EM algorithm for B and $(G_1, \dots, G_B)$ fixed : choice of $\boldsymbol{m} \Leftrightarrow$ choice of $\boldsymbol{\omega}$

The EM algorithm to achieve $\arg\max_{(\boldsymbol{\omega},\boldsymbol{\theta})} \ell_{pen}(\boldsymbol{\theta}_{\boldsymbol{m}}|\boldsymbol{m}, \mathbf{x})$, starting from $(\boldsymbol{\omega}^{[0]}, \boldsymbol{\theta}^{[0]})$ is at iteration $[r]$:

E-step Computation of the fuzzy partitions $t_{ibg}^{[r]} := \mathbb{E}[Z_{ibg}|\boldsymbol{x}_i, \boldsymbol{m}, \boldsymbol{\theta}^{[r-1]}]$, hence for $b = 1, \dots, B$, for $g = 1, \dots, G_b$, for $i = 1, \dots, n$

$$t_{ibg}^{[r]} = \frac{\pi_{bg}^{[r-1]} \prod_{j \in \Omega_b^{[r-1]}} p(x_{ij}|\boldsymbol{\alpha}_{jg}^{[r-1]})}{\sum_{k=1}^{G_b} \pi_{bk}^{[r-1]} \prod_{j \in \Omega_b^{[r-1]}} p(x_{ij}|\boldsymbol{\alpha}_{jg}^{[r-1]})},$$

M-step1 Updating the affectation of the variables to blocks

$$\omega_j^{[r]} = \underset{\omega_j \in \{1,\dots,B\}}{\arg\max} \left(\sum_{g=1}^{G_{\omega_j}} \max_{\boldsymbol{\alpha}_{jg} \in \Theta_j} Q(\boldsymbol{\alpha}_{jg}|\mathbf{x}_j, \mathbf{t}_{\omega_j g}^{[r]}) - \frac{\nu_j G_{\omega_j}}{2} \ln n \right),$$

M-step2 Updating the model parameters

$$\pi_{bg}^{[r]} = \frac{n_{bg}^{[r]}}{n} \text{ and } \boldsymbol{\alpha}_{jg}^{[r]} = \underset{\boldsymbol{\alpha}_{jg} \in \Theta_j}{\arg\max} Q(\boldsymbol{\alpha}_{jg}|\mathbf{x}_j, \mathbf{t}_{\omega_j^{[r]} g}^{[r]}).$$

Integrated complete-data likelihood

$$p(\mathbf{x}, \mathbf{z}|\boldsymbol{m}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{m}, \boldsymbol{\theta}) p(\boldsymbol{\theta}|\boldsymbol{m}) d\boldsymbol{\theta}.$$

Assumptions

- Independence between the prior distributions
- Standard conjugate priors
- Closed form of the complete-data integrated likelihood

MICL (maximum integrated complete-data likelihood) criterion

$$\text{MICL}(\boldsymbol{m}) = \ln p(\mathbf{x}, \mathbf{z}^\star_{\boldsymbol{m}}|\boldsymbol{m}) \text{ with } \mathbf{z}^\star_{\boldsymbol{m}} = \arg\max_{\mathbf{z}_{\boldsymbol{m}}} \ln p(\mathbf{x}, \mathbf{z}|\boldsymbol{m}).$$

Thus

$$(\boldsymbol{m}^\star, \mathbf{z}^\star_{\boldsymbol{m}^\star}) = \arg\max_{(\boldsymbol{m}, \mathbf{z}_{\boldsymbol{m}})} \ln p(\mathbf{x}, \mathbf{z}|\boldsymbol{m}).$$

Motivations

- Criteria based on the integrated complete-data likelihood are popular for model-based clustering
- Take into account the clustering purpose : model the data distribution and provide well-separated components

Optimisation of MICL over $(\mathbf{z}, \boldsymbol{\omega})$ for B and $G_1, \dots, G_B$ fixed

Starting at the initial value $\boldsymbol{\omega}^{[0]}$, each ω_j is uniformly sampled among $\{1, \dots, B\}$, the algorithm at iteration $[r]$ is

Partition step: find $\mathbf{z}_b^{[r]}$ such that for all $b = 1, \dots, B$

$$p(\mathbf{x}_{\{b\}}^{[r-1]}, \mathbf{z}_b^{[r]}) \geq p(\mathbf{x}_{\{b\}}^{[r-1]}, \mathbf{z}_b^{[r-1]}),$$

where $\mathbf{x}_{\{b\}}^{[r-1]} = (\mathbf{x}_j; \boldsymbol{\omega}^{[r-1]} = b)$.

Model step: find $\boldsymbol{\omega}^{[r]}$ such that for $j = 1, \dots, d$

$$\omega_j^{[r]} = \underset{b \in \{1,\dots,B\}}{\arg\max}\; p(\mathbf{x}_j | \mathbf{z}_b^{[r]}).$$

Data description

NBA teams for the season 2016/2017 described by 16 numerical variables[1]

- total minutes played (min)
- field goals made rate (fgmr)
- field goals attempted (fga)
- three-pointers made rate (3pmr)
- three-pointer attempted (3pa)
- free throws made (ftm)
- free throw attempted (fta)
- offensive rebounds (or)
- total rebounds (tr)
- assists (as)
- steals (st)
- turnovers (to)
- blocks (bk)
- personal fouls (pf)
- technical fouls (tc)
- points (pts)

Model selection with BIC

B	BIC	Time (s)	Block	G	variables
1	-1932	7	1	2	all the variables
2	-1915	47	1	3	fgmr, fga, 3pmr, 3pa, tr, as, to, pts
			2	1	min, ftmr, fta, orr, st, bk, pf, tc
3	-1909	170	1	2	fgmr, 3pmr, pf
			2	2	fga, 3pa, tr, as, st, to, pts
			3	1	min, ftmr, fta, orr, bk, tc

[1] http://www.dougstats.com/16-17RD.Team.Opp.txt

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Model parameters

First block: offensive vs defensive teams

Three features: field goals made rate, three points made rate and personal fouls

		fmgr	3pmr	pf
offensive teams: $(\pi_{11} = 0.57)$	mean	0.468	0.371	1628.042
high shooting ability	sd	0.009	0.010	76.138
low personal fouls				
defensive teams: $(\pi_{12} = 0.43)$	mean	0.446	0.342	1635.503
low shooting ability	sd	0.005	0.010	173.701
high personal fouls				

Second block: two better statistics teams for general performances vs others

Seven features: field goal attempted, 3 points attempted, total rebounds, assists, steals, turnovers and points

		fga	3pa	tr	as	st	to	pts
GS Warriors: $(\pi_{11} = 0.07)$	mean	7144	2934	3642	2281	728	1186	9481
Houston Rockets	sd	3	372	3	211	59	3	22
Other: $(\pi_{11} = 0.93)$	mean	6992	2162	3564	1825	626	1091	8600
teams	sd	183	262	141	131	45	105	259

Third block: Six features detected as irrelevant for clustering.

Data description

Data[1]

- 27 chemical and physical properties of three types of Italian wines: Barolo, Grignolino, Barbera
- Data collected during the time period of 1970–1979

Models selected by BIC

B	BIC	Time	Block	G	ARI
1	-6025.00	30	1	4	0.78
2	-5947.88	280	1	3	0.87
			2	4	0.16
3	-5921.42	1590	1	4	0.74
			2	4	0.20
			3	2	0.02
4	-5918.06	6065	1	4	0.75
			2	2	0.21
			3	3	0.02
			4	2	0.00

[1] available in the package pgmm

Model interpretation

Block 1: the type of wines (ARI=0.75)

19 variables: Alcohol, Sugar-free Extract, Tartaric Acid, Uronic Acids, Alcalinity of Ash, Calcium, Magnesium, Phosphate, Total Phenols, Flavanoids, Non-flavanoid Phenols, Proanthocyanins, Color Intensity, Hue, OD280/OD315 of Diluted Wines, OD280/OD315 of Flavanoids, Glycerol, 2-3-Butanediol, Proline

	Barolo	Grignolino	Barbera
Class 1	0	45	0
Class 2	0	5	48
Class 3	58	1	0
Class 4	1	20	0

Block 2: year of production

4 variables: Fixed Acidity, Malic Acid, pH, Total Nitrogen

	Year								
	1970	1971	1972	1973	1974	1975	1976	1978	1979
Class 1	8	25	4	27	31	3	1	0	0
Class 2	1	3	3	2	14	6	16	29	5

Conclusion

- Proposition of model-based clustering with several class variables, each one explaining the heterogeneity of a block of variables:
  - Find groups of variables producing the same clustering of the individuals
  - Interpret the clustering produced for each group of variables
- Model search performed simultaneously with parameters estimation
- Proposed model can be used in the heterogeneous data settings

Perspectives

- Consider the semi-supervised setting in the multi-partition framework for new partitions discovery: *i. e.* $\mathbf{z}_1$ known and $\mathbf{z}_2$ unknown.
- Extension to heterogeneous co-clustering by adding one level of latent variable to summarize the multi-partition by a single partition, while keeping the partition of the variables.
- Derive some k-means type multi-partition similary to Witten & Tibshirani (2010) in the variable selection framework to deal with the very high dimensional setting.